



Showcasing research from Professor Dheeraj Kumar's laboratory, Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee, India.

Taming of 4-azido-3,5-dinitropyrazole based energetic materials

4-Azido-3,5-dinitropyrazole (AzDNP) and its derivatives are attractive candidates as green energetic materials due to their excellent energetic properties and high nitrogen and oxygen contents. However, they are often more sensitive (primary explosives) and have poor thermal stability ( $T_d < 150\text{ }^{\circ}\text{C}$ ), attributed to the presence of azido functionality. In this work, we have tried to fine-tune the properties of 4-azido-3,5-dinitropyrazole by connecting it to 5-nitramino-1,2,4-oxadiazole moieties *via* *N*-methylene-*C* bridges and by energetic salts formation. The structure-property relationship was studied using Hirshfeld surface and Non-Covalent Interaction (NCI) analysis.

As featured in:



See Dheeraj Kumar *et al.*, *Mater. Adv.*, 2024, 5, 171.